cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3,4-dimethoxy, diacetate

Inchi: InChI=1S/C21H22O6/c1-12(22)26-20-15-10-11-17(24-4)19(25-5)18(15)14-8-6-7-9-16(14)

InchiKey: BMCSEJOBKZMRSX-RTWAWAEBSA-N

Formula: C21H22O6

SMILES: COc1ccc2c(c1OC)-c1ccccc1C(C)(OC(C)=O)C2OC(C)=O

Mol. weight [g/mol]: 370.40

Physical Properties

Property code	Value	Unit	Source
gf	-305.95	kJ/mol	Joback Method
hf	-729.77	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	3.767		Crippen Method
mcvol	274.990	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	948.62	K	Joback Method
tc	1181.31	K	Joback Method
tf	659.25	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.30	J/mol×K	948.62	Joback Method
cpg	892.13	J/mol×K	987.40	Joback Method
cpg	908.57	J/mol×K	1026.18	Joback Method
cpg	924.72	J/mol×K	1064.97	Joback Method
cpg	940.72	J/mol×K	1103.75	Joback Method
cpg	956.70	J/mol×K	1142.53	Joback Method
cpg	972.76	J/mol×K	1181.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume